



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:53 PM GMT

PDB ID : 4Z7I  
Title : Crystal structure of insulin regulated aminopeptidase in complex with ligand  
Authors : Mpakali, A.; Saridakis, E.; Harlos, K.; Zhao, Y.; Stratikos, E.  
Deposited on : 2015-04-07  
Resolution : 3.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

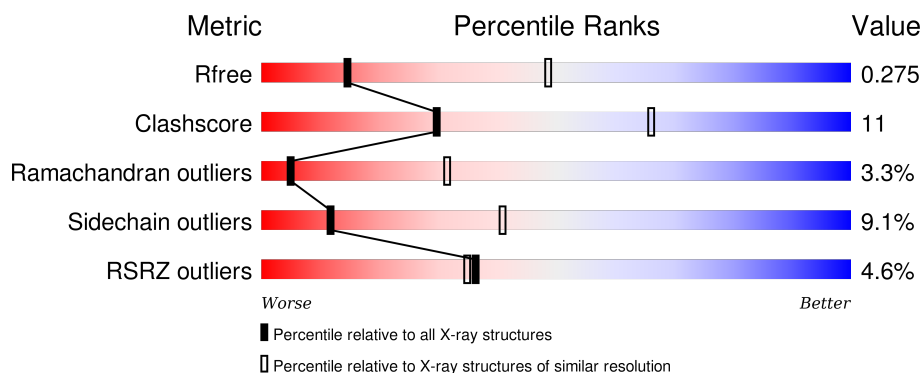
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	912	<div> <div>3%</div> <div>65%</div> <div>24%</div> <div>• • 6%</div> </div>
1	B	912	<div> <div>6%</div> <div>61%</div> <div>28%</div> <div>• 7%</div> </div>
2	C	10	<div> <div>60%</div> <div>30%</div> <div>10%</div> </div>
2	D	10	<div> <div>10%</div> <div>30%</div> <div>10%</div> <div>50%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	1113	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14358 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Leucyl-cystinyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	859	Total	C	N	O	S	0	0	0
			6947	4496	1132	1293	26			
1	B	852	Total	C	N	O	S	0	0	0
			6874	4448	1117	1284	25			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	initiating methionine	UNP Q9UIQ6
A	125	GLY	-	expression tag	UNP Q9UIQ6
A	126	ILE	-	expression tag	UNP Q9UIQ6
A	127	LEU	-	expression tag	UNP Q9UIQ6
A	128	PRO	-	expression tag	UNP Q9UIQ6
A	129	SER	-	expression tag	UNP Q9UIQ6
A	130	PRO	-	expression tag	UNP Q9UIQ6
A	131	GLY	-	expression tag	UNP Q9UIQ6
A	132	MET	-	expression tag	UNP Q9UIQ6
A	133	PRO	-	expression tag	UNP Q9UIQ6
A	134	ALA	-	expression tag	UNP Q9UIQ6
A	135	LEU	-	expression tag	UNP Q9UIQ6
A	136	LEU	-	expression tag	UNP Q9UIQ6
A	137	SER	-	expression tag	UNP Q9UIQ6
A	138	LEU	-	expression tag	UNP Q9UIQ6
A	139	VAL	-	expression tag	UNP Q9UIQ6
A	140	SER	-	expression tag	UNP Q9UIQ6
A	141	LEU	-	expression tag	UNP Q9UIQ6
A	142	LEU	-	expression tag	UNP Q9UIQ6
A	143	SER	-	expression tag	UNP Q9UIQ6
A	144	VAL	-	expression tag	UNP Q9UIQ6
A	145	LEU	-	expression tag	UNP Q9UIQ6
A	146	LEU	-	expression tag	UNP Q9UIQ6
A	147	MET	-	expression tag	UNP Q9UIQ6
A	148	GLY	-	expression tag	UNP Q9UIQ6

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	CYS	-	expression tag	UNP Q9UIQ6
A	150	VAL	-	expression tag	UNP Q9UIQ6
A	151	ALA	-	expression tag	UNP Q9UIQ6
A	152	GLU	-	expression tag	UNP Q9UIQ6
A	153	THR	-	expression tag	UNP Q9UIQ6
A	154	GLY	-	expression tag	UNP Q9UIQ6
A	1026	ARG	-	expression tag	UNP Q9UIQ6
A	1027	THR	-	expression tag	UNP Q9UIQ6
A	1028	GLU	-	expression tag	UNP Q9UIQ6
A	1029	THR	-	expression tag	UNP Q9UIQ6
A	1030	SER	-	expression tag	UNP Q9UIQ6
A	1031	GLN	-	expression tag	UNP Q9UIQ6
A	1032	VAL	-	expression tag	UNP Q9UIQ6
A	1033	ALA	-	expression tag	UNP Q9UIQ6
A	1034	PRO	-	expression tag	UNP Q9UIQ6
A	1035	ALA	-	expression tag	UNP Q9UIQ6
B	124	MET	-	initiating methionine	UNP Q9UIQ6
B	125	GLY	-	expression tag	UNP Q9UIQ6
B	126	ILE	-	expression tag	UNP Q9UIQ6
B	127	LEU	-	expression tag	UNP Q9UIQ6
B	128	PRO	-	expression tag	UNP Q9UIQ6
B	129	SER	-	expression tag	UNP Q9UIQ6
B	130	PRO	-	expression tag	UNP Q9UIQ6
B	131	GLY	-	expression tag	UNP Q9UIQ6
B	132	MET	-	expression tag	UNP Q9UIQ6
B	133	PRO	-	expression tag	UNP Q9UIQ6
B	134	ALA	-	expression tag	UNP Q9UIQ6
B	135	LEU	-	expression tag	UNP Q9UIQ6
B	136	LEU	-	expression tag	UNP Q9UIQ6
B	137	SER	-	expression tag	UNP Q9UIQ6
B	138	LEU	-	expression tag	UNP Q9UIQ6
B	139	VAL	-	expression tag	UNP Q9UIQ6
B	140	SER	-	expression tag	UNP Q9UIQ6
B	141	LEU	-	expression tag	UNP Q9UIQ6
B	142	LEU	-	expression tag	UNP Q9UIQ6
B	143	SER	-	expression tag	UNP Q9UIQ6
B	144	VAL	-	expression tag	UNP Q9UIQ6
B	145	LEU	-	expression tag	UNP Q9UIQ6
B	146	LEU	-	expression tag	UNP Q9UIQ6
B	147	MET	-	expression tag	UNP Q9UIQ6
B	148	GLY	-	expression tag	UNP Q9UIQ6
B	149	CYS	-	expression tag	UNP Q9UIQ6

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	150	VAL	-	expression tag	UNP Q9UIQ6
B	151	ALA	-	expression tag	UNP Q9UIQ6
B	152	GLU	-	expression tag	UNP Q9UIQ6
B	153	THR	-	expression tag	UNP Q9UIQ6
B	154	GLY	-	expression tag	UNP Q9UIQ6
B	1026	ARG	-	expression tag	UNP Q9UIQ6
B	1027	THR	-	expression tag	UNP Q9UIQ6
B	1028	GLU	-	expression tag	UNP Q9UIQ6
B	1029	THR	-	expression tag	UNP Q9UIQ6
B	1030	SER	-	expression tag	UNP Q9UIQ6
B	1031	GLN	-	expression tag	UNP Q9UIQ6
B	1032	VAL	-	expression tag	UNP Q9UIQ6
B	1033	ALA	-	expression tag	UNP Q9UIQ6
B	1034	PRO	-	expression tag	UNP Q9UIQ6
B	1035	ALA	-	expression tag	UNP Q9UIQ6

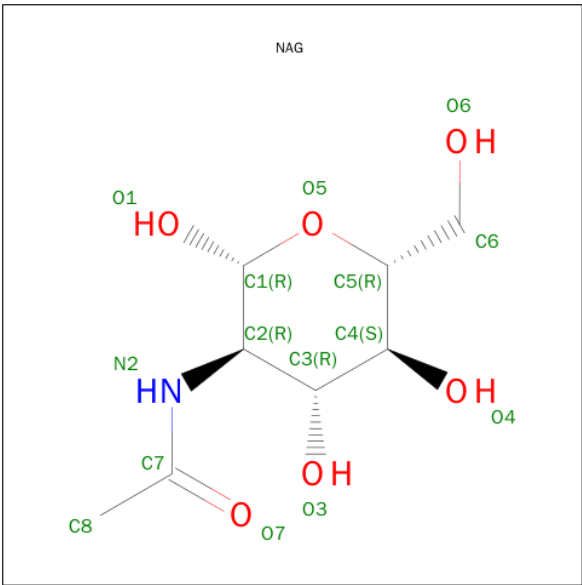
- Molecule 2 is a protein called DG025 transition-state analogue enzyme inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			87	58	15	13	1			
2	D	5	Total	C	N	O	P	0	0	0
			45	31	7	6	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



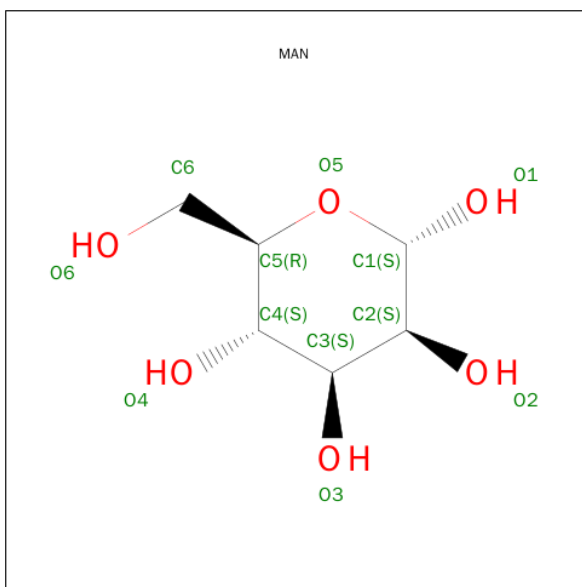
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

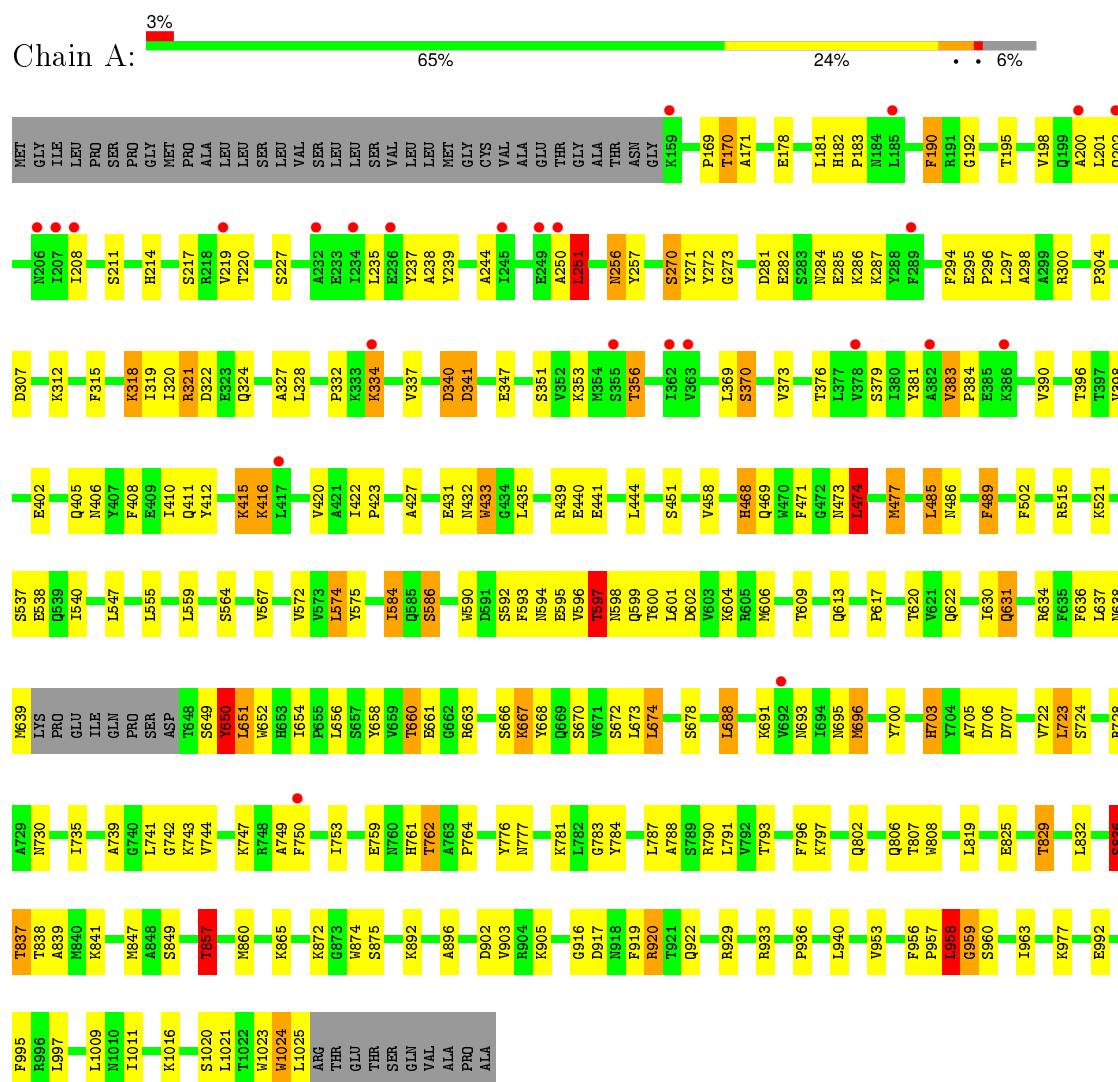
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	6	Total	O	0	0
			6	6		
6	C	1	Total	O	0	0
			1	1		

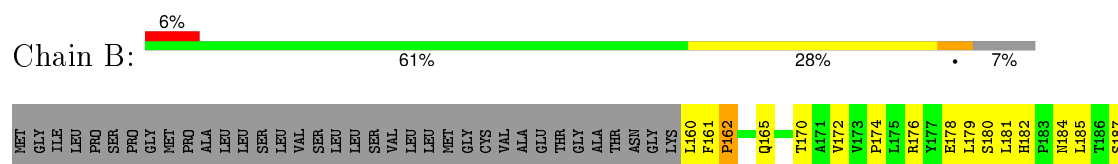
### 3 Residue-property plots

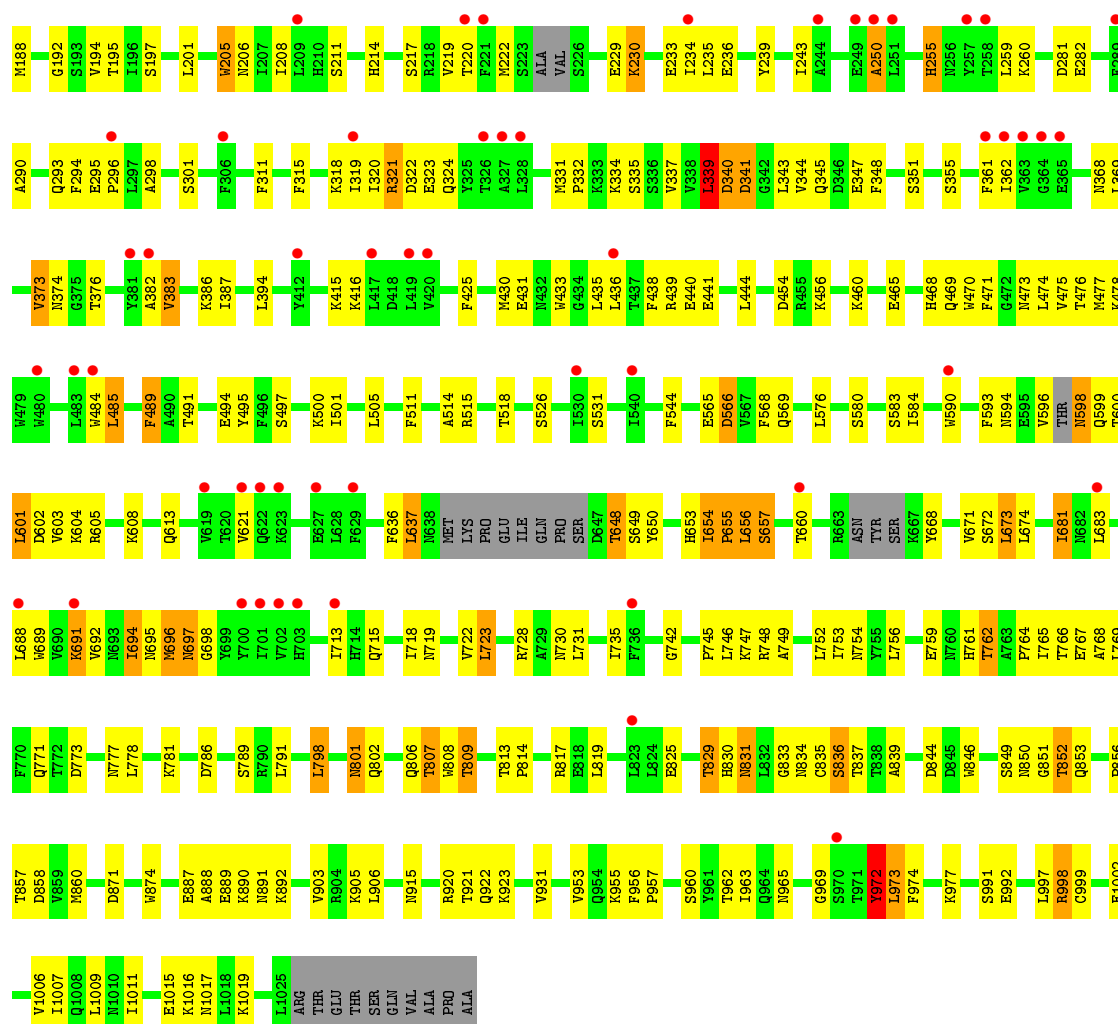
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Leucyl-cystinyl aminopeptidase



- Molecule 1: Leucyl-cystinyl aminopeptidase





- Molecule 2: DG025 transition-state analogue enzyme inhibitor

Chain C:



- Molecule 2: DG025 transition-state analogue enzyme inhibitor

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.52Å 256.35Å 73.06Å 90.00° 111.58° 90.00°	Depositor
Resolution (Å)	128.18 – 3.31 128.17 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (128.18-3.31) 99.9 (128.17-3.31)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.211 , 0.270 0.223 , 0.275	Depositor DCC
$R_{free}$ test set	1676 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	127.3	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 85.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 34760 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14358	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2X0, ZN, 4L8, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/7117	0.49	1/9654 (0.0%)
1	B	0.26	0/7038	0.52	1/9543 (0.0%)
2	C	0.27	0/68	0.69	0/87
2	D	0.19	0/24	0.25	0/30
All	All	0.26	0/14247	0.50	2/19314 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	339	LEU	CA-CB-CG	7.86	133.38	115.30
1	A	251	LEU	CA-CB-CG	6.00	129.09	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	596	VAL	Peptide
1	A	598	ASN	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6947	0	6829	149	0
1	B	6874	0	6745	164	0
2	C	87	0	83	2	0
2	D	45	0	44	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	210	0	190	2	0
4	B	168	0	154	5	0
5	A	11	0	10	1	0
6	A	7	0	0	0	0
6	B	6	0	0	0	0
6	C	1	0	0	0	0
All	All	14358	0	14055	318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (318) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:ARG:HD3	1:A:1025:LEU:HD22	1.52	0.89
1:B:655:PRO:HA	1:B:656:LEU:HB2	1.61	0.82
1:B:331:MET:HG3	1:B:351:SER:HA	1.65	0.78
1:A:597:THR:H	1:A:599:GLN:H	1.35	0.75
1:B:691:LYS:HE2	1:B:731:LEU:HG	1.68	0.74
1:B:178:GLU:HB3	1:B:195:THR:HB	1.68	0.73
1:B:835:CYS:SG	1:B:836:SER:N	2.61	0.73
1:A:307:ASP:HA	1:A:356:THR:HG21	1.71	0.72
1:B:833:GLY:O	1:B:835:CYS:N	2.22	0.71
1:A:321:ARG:HG2	1:A:327:ALA:HB2	1.72	0.71
1:A:836:SER:O	1:A:838:THR:N	2.24	0.71
1:B:696:MET:O	1:B:698:GLY:N	2.20	0.71
1:B:594:ASN:ND2	1:B:602:ASP:O	2.21	0.71
1:B:294:PHE:HA	1:B:298:ALA:HB3	1.74	0.69
1:B:769:LEU:O	1:B:773:ASP:HB2	1.93	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:THR:HG23	1:A:601:LEU:HB3	1.73	0.69
1:B:921:THR:HG21	1:B:955:LYS:HD3	1.75	0.68
1:A:415:LYS:HE2	1:A:415:LYS:H	1.57	0.68
1:A:294:PHE:HA	1:A:298:ALA:HB3	1.76	0.67
1:B:657:SER:HB3	1:B:671:VAL:HG12	1.76	0.66
1:A:297:LEU:HD23	1:A:300:ARG:HH12	1.60	0.65
1:B:335:SER:O	1:B:347:GLU:N	2.29	0.65
1:B:182:HIS:HB2	1:B:320:ILE:HD12	1.79	0.65
1:B:621:VAL:HG21	1:B:692:VAL:HG21	1.79	0.65
1:B:762:THR:HB	1:B:819:LEU:HB2	1.79	0.64
1:A:688:LEU:H	1:A:688:LEU:HD23	1.63	0.64
1:A:178:GLU:HB3	1:A:195:THR:HB	1.78	0.64
1:A:630:ILE:HG21	1:A:656:LEU:HD11	1.78	0.64
1:A:696:MET:SD	1:A:730:ASN:ND2	2.71	0.64
1:B:475:VAL:HG12	1:B:584:ILE:HG12	1.80	0.64
1:B:236:GLU:HG2	1:B:243:ILE:HG22	1.79	0.64
1:B:718:ILE:HG13	1:B:719:ASN:H	1.61	0.63
1:A:405:GLN:HG2	1:A:411:GLN:HA	1.78	0.63
1:A:762:THR:HB	1:A:819:LEU:HB2	1.80	0.63
1:B:957:PRO:HG2	1:B:960:SER:HB2	1.81	0.62
1:A:672:SER:OG	1:A:673:LEU:N	2.32	0.62
1:A:281:ASP:OD1	1:A:282:GLU:N	2.33	0.62
1:A:341:ASP:N	1:A:341:ASP:OD1	2.33	0.62
1:B:340:ASP:N	1:B:340:ASP:OD1	2.27	0.62
1:A:637:LEU:HB3	1:A:1009:LEU:HD21	1.82	0.61
1:A:847:MET:HE2	1:A:872:LYS:HE2	1.81	0.61
2:C:2:4L8:O	2:C:3:LYS:HB2	2.01	0.61
1:A:477:MET:SD	1:A:486:ASN:ND2	2.74	0.60
1:B:321:ARG:NH2	1:B:323:GLU:O	2.35	0.60
1:B:219:VAL:HG21	1:B:234:ILE:HD11	1.83	0.60
1:B:576:LEU:O	1:B:580:SER:OG	2.15	0.60
1:A:270:SER:OG	1:A:271:TYR:N	2.33	0.60
1:A:433:TRP:HZ2	1:A:474:LEU:HD12	1.66	0.60
1:B:972:TYR:C	1:B:974:PHE:H	2.05	0.59
1:A:599:GLN:O	1:A:600:THR:OG1	2.19	0.59
1:B:319:ILE:HD11	1:B:361:PHE:HB2	1.84	0.59
1:B:179:LEU:O	1:B:318:LYS:N	2.29	0.59
1:A:451:SER:HB3	1:A:857:THR:HB	1.84	0.58
1:A:903:VAL:HG13	1:A:940:LEU:HD22	1.86	0.58
1:A:957:PRO:O	1:A:959:GLY:N	2.37	0.57
1:B:681:ILE:HG22	4:B:1107:NAG:H82	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:GLU:O	1:A:829:THR:OG1	2.20	0.57
1:B:825:GLU:O	1:B:829:THR:OG1	2.22	0.57
1:B:281:ASP:OD1	1:B:282:GLU:N	2.36	0.57
1:B:339:LEU:HD22	1:B:343:LEU:H	1.70	0.56
1:A:660:THR:OG1	1:A:661:GLU:N	2.38	0.56
1:A:728:ARG:NH1	1:A:759:GLU:OE2	2.38	0.56
1:A:312:LYS:NZ	1:A:474:LEU:O	2.34	0.56
1:A:272:TYR:CZ	1:A:298:ALA:HB2	2.40	0.56
1:B:637:LEU:HD13	1:B:1009:LEU:HD11	1.86	0.55
1:A:703:HIS:HD2	1:A:743:LYS:HD2	1.70	0.55
1:B:695:ASN:HB2	1:B:697:ASN:ND2	2.22	0.55
1:A:370:SER:HB3	1:A:379:SER:HB3	1.88	0.55
1:B:205:TRP:NE1	1:B:250:ALA:HB2	2.21	0.55
1:A:836:SER:O	1:A:839:ALA:N	2.38	0.55
1:A:691:LYS:NZ	1:A:693:ASN:O	2.35	0.55
1:A:235:LEU:HB2	1:A:244:ALA:HB3	1.88	0.55
1:B:335:SER:OG	1:B:347:GLU:OE1	2.16	0.55
1:B:315:PHE:N	1:B:351:SER:OG	2.39	0.54
1:B:956:PHE:HB2	1:B:963:ILE:HD13	1.89	0.54
1:B:425:PHE:O	1:B:439:ARG:NE	2.40	0.54
1:A:169:PRO:HG3	1:A:208:ILE:HD13	1.89	0.54
1:A:237:TYR:O	1:A:239:TYR:N	2.38	0.54
1:A:597:THR:H	1:A:599:GLN:N	2.06	0.54
1:B:728:ARG:NH1	1:B:759:GLU:OE2	2.41	0.54
1:A:564:SER:HB3	1:A:567:VAL:HG23	1.89	0.54
1:A:634:ARG:HD2	1:A:650:TYR:CE1	2.43	0.53
1:B:746:LEU:HD22	1:B:1017:ASN:HB3	1.89	0.53
1:A:929:ARG:O	1:A:933:ARG:HG3	2.09	0.53
1:B:713:ILE:HG23	1:B:752:LEU:HA	1.91	0.53
1:B:334:LYS:H	1:B:348:PHE:HA	1.74	0.53
1:A:695:ASN:OD1	1:A:724:SER:OG	2.15	0.53
1:B:373:VAL:HG13	1:B:374:ASN:H	1.73	0.52
1:A:622:GLN:OE1	1:A:631:GLN:NE2	2.42	0.52
1:A:956:PHE:HB2	1:A:963:ILE:HD13	1.91	0.52
1:B:722:VAL:HG23	1:B:723:LEU:HG	1.90	0.52
1:A:658:TYR:CZ	1:A:670:SER:HB3	2.45	0.52
2:D:3:LYS:O	2:D:4:HIS:ND1	2.42	0.52
1:A:957:PRO:HG2	1:A:960:SER:HB3	1.90	0.52
1:B:179:LEU:HD13	1:B:194:VAL:HG22	1.92	0.52
1:A:281:ASP:OD2	1:A:287:LYS:HE2	2.10	0.52
1:B:332:PRO:HG2	1:B:415:LYS:HB3	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLN:OE1	1:A:473:ASN:ND2	2.42	0.52
1:B:807:THR:OG1	1:B:809:THR:OG1	2.27	0.52
1:A:777:ASN:O	1:A:781:LYS:HG2	2.10	0.52
1:B:801:ASN:OD1	1:B:801:ASN:N	2.30	0.52
1:A:485:LEU:HD21	1:A:586:SER:HA	1.91	0.51
1:B:194:VAL:O	1:B:260:LYS:HA	2.11	0.51
1:A:402:GLU:O	1:A:406:ASN:ND2	2.42	0.51
1:B:655:PRO:HA	1:B:656:LEU:CB	2.37	0.51
1:A:992:GLU:HA	1:A:995:PHE:HB3	1.91	0.51
1:A:613:GLN:HE22	1:A:650:TYR:HA	1.76	0.51
1:A:761:HIS:O	1:A:764:PRO:HD2	2.11	0.51
1:A:200:ALA:HB2	1:A:251:LEU:HD23	1.93	0.51
1:B:439:ARG:NH2	1:B:441:GLU:OE1	2.43	0.51
1:A:874:TRP:CD2	1:A:905:LYS:HD3	2.45	0.51
1:B:544:PHE:CE1	2:D:1:2X0:H15	2.46	0.51
1:A:485:LEU:O	1:A:489:PHE:HB2	2.11	0.50
1:A:936:PRO:HA	1:B:903:VAL:HG21	1.92	0.50
1:B:544:PHE:CD2	2:D:1:2X0:H14	2.47	0.50
1:B:745:PRO:HG2	1:B:748:ARG:HB2	1.92	0.50
4:B:1111:NAG:H62	4:B:1112:NAG:C7	2.41	0.50
1:B:383:VAL:HG12	1:B:386:LYS:H	1.77	0.50
1:B:835:CYS:O	1:B:837:THR:N	2.45	0.50
1:B:598:ASN:O	1:B:598:ASN:ND2	2.29	0.50
1:A:515:ARG:NH2	1:A:696:MET:O	2.45	0.50
1:B:874:TRP:CD2	1:B:905:LYS:HD3	2.46	0.50
1:A:315:PHE:HB2	1:A:351:SER:HB3	1.92	0.50
1:A:379:SER:HB2	1:A:381:TYR:HE1	1.76	0.49
1:A:750:PHE:CZ	1:A:791:LEU:HD11	2.47	0.49
1:B:851:GLY:O	1:B:853:GLN:N	2.45	0.49
1:B:430:MET:HG3	1:B:431:GLU:N	2.26	0.49
1:A:590:TRP:HB3	1:A:604:LYS:HB2	1.94	0.49
1:B:802:GLN:O	1:B:806:GLN:HG2	2.13	0.49
1:B:718:ILE:HG13	1:B:719:ASN:N	2.28	0.49
1:B:219:VAL:HG11	1:B:234:ILE:HD11	1.93	0.49
1:B:318:LYS:HG2	1:B:347:GLU:HA	1.94	0.49
1:B:290:ALA:O	1:B:362:ILE:HG23	2.12	0.49
1:A:340:ASP:OD1	1:A:340:ASP:N	2.41	0.49
1:A:477:MET:HA	1:A:584:ILE:HG22	1.94	0.49
1:B:596:VAL:HG21	1:B:601:LEU:HB3	1.94	0.49
1:A:802:GLN:O	1:A:806:GLN:HG2	2.13	0.49
1:A:916:GLY:HA2	1:A:919:PHE:O	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:OG1	1:A:202:GLN:OE1	2.31	0.48
1:A:902:ASP:OD2	1:A:905:LYS:NZ	2.46	0.48
1:B:222:MET:HA	1:B:229:GLU:O	2.13	0.48
1:A:373:VAL:HG11	1:A:398:VAL:HG13	1.96	0.48
1:B:887:GLU:HA	1:B:890:LYS:HB2	1.94	0.48
1:B:672:SER:OG	1:B:672:SER:O	2.29	0.48
1:A:620:THR:HG22	1:A:622:GLN:HE22	1.78	0.48
1:B:997:LEU:O	1:B:999:CYS:N	2.41	0.48
1:A:622:GLN:HG3	1:A:705:ALA:HB2	1.96	0.48
1:B:440:GLU:O	1:B:444:LEU:HG	2.14	0.48
1:A:318:LYS:HD3	1:A:347:GLU:HG3	1.95	0.48
1:B:767:GLU:OE2	1:B:771:GLN:NE2	2.40	0.47
1:A:237:TYR:C	1:A:239:TYR:H	2.17	0.47
1:B:742:GLY:HA3	1:B:1016:LYS:HD2	1.95	0.47
1:B:656:LEU:HD13	1:B:674:LEU:HB3	1.96	0.47
1:A:332:PRO:HG3	1:A:416:LYS:HG2	1.96	0.47
1:B:696:MET:C	1:B:698:GLY:H	2.13	0.47
1:B:456:LYS:O	1:B:460:LYS:HB2	2.14	0.47
1:A:790:ARG:HD3	1:A:1025:LEU:CD2	2.36	0.47
1:A:977:LYS:HD3	1:A:1011:ILE:HD13	1.95	0.47
1:A:747:LYS:HG3	1:A:1024:TRP:CZ2	2.50	0.47
1:B:813:THR:O	1:B:817:ARG:HG2	2.14	0.47
1:A:865:LYS:HG2	1:A:896:ALA:HA	1.96	0.47
1:B:181:LEU:HD23	1:B:192:GLY:HA3	1.97	0.47
1:B:603:VAL:HG13	1:B:605:ARG:HG2	1.96	0.47
1:B:478:LYS:HA	1:B:583:SER:HB3	1.97	0.47
1:A:477:MET:N	1:A:477:MET:SD	2.88	0.47
1:A:396:THR:HG23	1:A:502:PHE:CZ	2.50	0.47
1:B:1002:GLU:O	1:B:1006:VAL:HG23	2.16	0.47
1:B:324:GLN:N	1:B:324:GLN:OE1	2.46	0.47
1:B:972:TYR:O	1:B:973:LEU:HB2	2.15	0.46
1:A:469:GLN:O	1:A:473:ASN:HB2	2.15	0.46
1:A:666:SER:O	1:A:668:TYR:N	2.48	0.46
1:B:321:ARG:NE	1:B:322:ASP:O	2.46	0.46
1:B:849:SER:HB3	1:B:852:THR:HB	1.97	0.46
1:B:515:ARG:HH21	1:B:696:MET:HB3	1.81	0.46
1:A:471:PHE:HZ	1:A:572:VAL:HG13	1.81	0.46
1:B:491:THR:O	1:B:494:GLU:HB3	2.14	0.46
1:B:485:LEU:O	1:B:489:PHE:HB2	2.16	0.46
1:A:256:ASN:OD1	1:A:256:ASN:N	2.49	0.46
1:A:381:TYR:OH	4:A:1108:NAG:H82	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:SER:HB3	1:A:837:THR:H	1.55	0.46
1:A:211:SER:HB2	1:A:304:PRO:HB3	1.97	0.46
1:A:273:GLY:HA2	1:A:298:ALA:HB1	1.98	0.46
1:A:297:LEU:HD11	1:A:540:ILE:HD13	1.98	0.45
1:A:574:LEU:HD22	1:A:595:GLU:HG3	1.99	0.45
1:A:334:LYS:HB3	1:A:334:LYS:HE3	1.51	0.45
1:A:181:LEU:HD23	1:A:192:GLY:HA3	1.98	0.45
1:B:654:ILE:HA	1:B:655:PRO:HD3	1.76	0.45
1:B:180:SER:HB2	1:B:318:LYS:HE3	1.99	0.45
4:A:1113:NAG:O3	5:A:1114:MAN:H2	2.16	0.45
1:B:753:ILE:HG23	1:B:756:LEU:HD13	1.98	0.45
1:B:182:HIS:HD1	1:B:320:ILE:HB	1.81	0.45
1:A:555:LEU:O	1:A:559:LEU:N	2.41	0.45
1:B:694:ILE:C	1:B:696:MET:H	2.20	0.45
1:A:183:PRO:HA	1:A:190:PHE:HB3	1.98	0.45
1:B:696:MET:SD	1:B:730:ASN:ND2	2.89	0.45
1:B:745:PRO:HB2	1:B:747:LYS:HG2	1.99	0.45
1:B:187:SER:OG	1:B:188:MET:N	2.49	0.45
1:A:597:THR:OG1	1:A:597:THR:O	2.31	0.45
1:B:476:THR:O	1:B:584:ILE:HG13	2.17	0.45
1:A:379:SER:HB2	1:A:381:TYR:CE1	2.51	0.45
1:A:369:LEU:HD23	1:A:390:VAL:HG23	1.97	0.45
1:B:1007:ILE:O	1:B:1011:ILE:HG13	2.17	0.45
1:B:179:LEU:CD1	1:B:194:VAL:HG22	2.47	0.45
1:B:637:LEU:HB2	1:B:1009:LEU:HD21	1.98	0.45
1:A:182:HIS:HB2	1:A:320:ILE:HD12	1.98	0.45
1:A:742:GLY:HA3	1:A:1016:LYS:HE2	1.98	0.45
1:B:906:LEU:HD22	1:B:931:VAL:HG22	1.97	0.44
1:A:594:ASN:OD1	1:A:604:LYS:HG2	2.16	0.44
1:B:689:TRP:CD1	1:B:715:GLN:HG3	2.52	0.44
1:B:766:THR:O	1:B:769:LEU:HG	2.17	0.44
1:A:750:PHE:CD1	1:A:753:ILE:HD11	2.53	0.44
1:A:383:VAL:HG22	1:A:384:PRO:HD2	1.99	0.44
1:A:630:ILE:HB	1:A:674:LEU:HD13	2.00	0.44
1:B:234:ILE:HG22	1:B:235:LEU:N	2.33	0.44
1:B:759:GLU:OE2	1:B:761:HIS:HB2	2.18	0.44
1:A:857:THR:O	1:A:892:LYS:NZ	2.50	0.44
1:A:181:LEU:HB2	1:A:319:ILE:HG22	2.00	0.44
1:A:538:GLU:OE1	1:A:538:GLU:N	2.50	0.44
1:B:844:ASP:O	1:B:846:TRP:N	2.48	0.44
1:A:328:LEU:HD11	1:A:381:TYR:CD2	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:VAL:N	1:B:345:GLN:O	2.33	0.44
1:B:161:PHE:HA	1:B:235:LEU:HD21	2.00	0.44
1:B:174:PRO:HD2	1:B:311:PHE:HD2	1.82	0.44
1:B:211:SER:HB3	1:B:243:ILE:HG23	1.99	0.44
1:A:575:TYR:OH	1:A:584:ILE:HG13	2.18	0.44
1:A:251:LEU:HB2	1:A:257:TYR:CE1	2.53	0.44
1:B:185:LEU:H	4:B:1102:NAG:H82	1.83	0.43
1:A:776:TYR:CD2	1:A:788:ALA:HB1	2.53	0.43
1:A:422:ILE:HA	1:A:423:PRO:HD3	1.77	0.43
1:A:1020:SER:HA	1:A:1023:TRP:HE1	1.83	0.43
1:A:321:ARG:HG3	1:A:321:ARG:H	1.60	0.43
1:A:837:THR:O	1:A:841:LYS:N	2.41	0.43
1:B:594:ASN:O	1:B:600:THR:HG22	2.19	0.43
1:B:777:ASN:O	1:B:781:LYS:HG2	2.18	0.43
1:B:514:ALA:O	1:B:518:THR:OG1	2.31	0.43
1:A:658:TYR:CE2	1:A:670:SER:HB3	2.53	0.43
1:A:537:SER:HA	1:A:540:ILE:HD12	2.01	0.43
1:B:471:PHE:CZ	1:B:576:LEU:HD11	2.53	0.43
1:B:817:ARG:HB2	1:B:858:ASP:OD2	2.19	0.43
1:A:376:THR:HG21	1:A:412:TYR:HD2	1.84	0.43
1:A:1024:TRP:HB3	1:A:1025:LEU:H	1.43	0.43
1:B:162:PRO:HG2	1:B:208:ILE:HD11	2.00	0.43
1:A:735:ILE:HG12	1:A:749:ALA:HA	2.01	0.43
1:B:648:THR:HA	1:B:649:SER:HA	1.80	0.43
1:B:850:ASN:OD1	4:B:1108:NAG:H2	2.19	0.43
1:A:201:LEU:HA	1:A:201:LEU:HD23	1.80	0.43
1:A:857:THR:HA	1:A:860:MET:HB2	2.01	0.43
1:A:617:PRO:HG2	1:A:700:TYR:HB3	2.01	0.43
1:B:891:ASN:HD21	1:B:923:LYS:HE2	1.83	0.43
1:A:198:VAL:O	1:A:257:TYR:N	2.46	0.43
2:C:3:LYS:HD3	2:C:3:LYS:HA	1.68	0.42
1:A:584:ILE:HD13	1:A:584:ILE:HA	1.77	0.42
1:B:920:ARG:HH22	1:B:923:LYS:NZ	2.17	0.42
1:B:998:ARG:HE	1:B:998:ARG:HB3	1.65	0.42
1:A:592:SER:HA	1:A:595:GLU:HG2	2.01	0.42
1:B:735:ILE:HG12	1:B:749:ALA:HA	2.00	0.42
1:B:888:ALA:O	1:B:892:LYS:HG3	2.19	0.42
1:B:478:LYS:N	1:B:584:ILE:O	2.48	0.42
1:A:408:PHE:O	1:A:410:ILE:HD12	2.20	0.42
1:B:544:PHE:CG	2:D:1:2X0:H14	2.55	0.42
1:B:214:HIS:NE2	1:B:301:SER:O	2.52	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:THR:HG21	1:B:683:LEU:HD21	2.01	0.42
1:B:723:LEU:HD13	1:B:728:ARG:HG3	2.02	0.42
1:B:332:PRO:HG3	1:B:416:LYS:HG2	2.01	0.42
1:A:920:ARG:NH1	1:A:922:GLN:OE1	2.52	0.42
1:B:830:HIS:O	1:B:831:ASN:HB2	2.19	0.42
1:B:484:TRP:HE1	1:B:531:SER:HG	1.66	0.42
1:B:469:GLN:O	1:B:473:ASN:HB2	2.20	0.42
1:A:312:LYS:HB3	1:A:353:LYS:HG2	2.02	0.42
2:D:2:4L8:O	2:D:3:LYS:HB2	2.20	0.41
1:B:860:MET:SD	1:B:889:GLU:HG3	2.60	0.41
1:A:654:ILE:O	1:A:673:LEU:HA	2.20	0.41
1:B:229:GLU:HG2	1:B:230:LYS:HZ3	1.85	0.41
1:B:856:PRO:O	1:B:858:ASP:N	2.53	0.41
1:A:432:ASN:HB2	1:A:435:LEU:O	2.21	0.41
1:A:440:GLU:O	1:A:444:LEU:HG	2.20	0.41
1:B:438:PHE:CE1	1:B:465:GLU:HG3	2.54	0.41
1:B:495:TYR:CD1	1:B:511:PHE:HB2	2.54	0.41
1:A:431:GLU:HG3	1:A:468:HIS:HB3	2.02	0.41
1:B:590:TRP:HB3	1:B:604:LYS:HB2	2.03	0.41
1:A:295:GLU:HA	1:A:296:PRO:HA	1.66	0.41
1:B:176:ARG:HB3	1:B:197:SER:HB2	2.02	0.41
1:B:965:ASN:O	1:B:969:GLY:N	2.52	0.41
1:B:694:ILE:O	1:B:696:MET:N	2.43	0.41
1:B:956:PHE:HA	1:B:957:PRO:HD2	1.82	0.41
1:B:673:LEU:O	1:B:673:LEU:HD23	2.20	0.41
1:A:953:VAL:HG22	1:A:958:LEU:HD13	2.03	0.41
1:B:594:ASN:N	1:B:594:ASN:OD1	2.52	0.41
1:B:778:LEU:HD23	1:B:973:LEU:HA	2.03	0.41
1:A:211:SER:OG	1:A:214:HIS:ND1	2.46	0.41
1:B:920:ARG:NH2	1:B:922:GLN:OE1	2.47	0.41
1:A:722:VAL:HG23	1:A:723:LEU:HG	2.02	0.41
1:A:808:TRP:CH2	1:A:839:ALA:HB2	2.56	0.41
1:A:728:ARG:HD2	1:A:759:GLU:OE1	2.21	0.41
1:A:427:ALA:HB3	1:A:439:ARG:HG2	2.02	0.41
1:A:285:GLU:OE2	1:A:287:LYS:NZ	2.50	0.40
1:B:368:ASN:OD1	4:B:1106:NAG:N2	2.55	0.40
1:B:808:TRP:CH2	1:B:839:ALA:HB2	2.56	0.40
1:A:784:TYR:HB3	1:A:787:LEU:HB2	2.04	0.40
1:A:796:PHE:HB2	1:A:832:LEU:HD13	2.02	0.40
1:B:1015:GLU:O	1:B:1019:LYS:HE2	2.21	0.40
1:B:754:ASN:HA	1:B:798:LEU:HD21	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLN:CD	1:B:324:GLN:H	2.24	0.40
1:B:500:LYS:HA	1:B:500:LYS:HD3	1.88	0.40
1:B:694:ILE:HG22	1:B:695:ASN:N	2.37	0.40
1:A:617:PRO:HD3	1:A:652:TRP:CD2	2.57	0.40
1:A:739:ALA:HA	1:A:744:VAL:O	2.21	0.40
1:B:565:GLU:O	1:B:566:ASP:OD1	2.40	0.40
1:B:295:GLU:HA	1:B:296:PRO:HA	1.67	0.40
1:B:331:MET:CG	1:B:351:SER:HA	2.42	0.40
1:B:470:TRP:HD1	1:B:576:LEU:HD23	1.86	0.40
1:A:956:PHE:HA	1:A:957:PRO:HD2	1.93	0.40
1:B:648:THR:HG22	1:B:649:SER:HA	2.03	0.40
1:B:438:PHE:CZ	1:B:465:GLU:HG3	2.56	0.40
1:B:505:LEU:HA	1:B:814:PRO:HG2	2.03	0.40
1:B:161:PHE:HD1	1:B:235:LEU:HG	1.86	0.40
1:B:339:LEU:CD2	1:B:343:LEU:H	2.34	0.40
1:A:613:GLN:NE2	1:A:650:TYR:HA	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	855/912 (94%)	762 (89%)	71 (8%)	22 (3%)	7	37
1	B	842/912 (92%)	723 (86%)	87 (10%)	32 (4%)	4	27
2	C	7/10 (70%)	1 (14%)	3 (43%)	3 (43%)	0	0
2	D	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
All	All	1706/1844 (92%)	1487 (87%)	162 (10%)	57 (3%)	5	31

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ALA
1	A	217	SER
1	A	238	ALA
1	A	663	ARG
1	A	836	SER
1	A	837	THR
1	A	958	LEU
1	B	373	VAL
1	B	569	GLN
1	B	655	PRO
1	B	656	LEU
1	B	673	LEU
1	B	834	ASN
1	B	852	THR
1	B	972	TYR
2	C	9	PHE
1	A	250	ALA
1	A	474	LEU
1	A	649	SER
1	A	667	LYS
1	A	849	SER
1	B	255	HIS
1	B	341	ASP
1	B	344	VAL
1	B	387	ILE
1	B	474	LEU
1	B	566	ASP
1	B	599	GLN
1	B	601	LEU
1	B	694	ILE
1	B	696	MET
1	B	697	ASN
1	B	998	ARG
1	A	638	ASN
1	A	1024	TRP
1	B	230	LYS
1	B	250	ALA
1	B	382	ALA
1	B	836	SER
1	B	857	THR
2	C	3	LYS
1	A	227	SER
1	A	597	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	650	TYR
1	A	651	LEU
1	A	783	GLY
1	A	959	GLY
1	B	217	SER
1	B	657	SER
2	C	5	HIS
1	A	696	MET
1	A	857	THR
1	B	768	ALA
1	B	831	ASN
1	B	764	PRO
1	B	765	ILE
1	B	162	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	761/813 (94%)	692 (91%)	69 (9%)	12	41
1	B	752/813 (92%)	684 (91%)	68 (9%)	12	42
2	C	6/7 (86%)	6 (100%)	0	100	100
2	D	2/7 (29%)	1 (50%)	1 (50%)	0	0
All	All	1521/1640 (93%)	1383 (91%)	138 (9%)	12	41

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	THR
1	A	190	PHE
1	A	219	VAL
1	A	220	THR
1	A	251	LEU
1	A	256	ASN
1	A	270	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	284	ASN
1	A	286	LYS
1	A	318	LYS
1	A	321	ARG
1	A	322	ASP
1	A	324	GLN
1	A	334	LYS
1	A	337	VAL
1	A	340	ASP
1	A	341	ASP
1	A	356	THR
1	A	370	SER
1	A	383	VAL
1	A	415	LYS
1	A	416	LYS
1	A	420	VAL
1	A	433	TRP
1	A	441	GLU
1	A	458	VAL
1	A	468	HIS
1	A	474	LEU
1	A	477	MET
1	A	485	LEU
1	A	489	PHE
1	A	521	LYS
1	A	547	LEU
1	A	574	LEU
1	A	584	ILE
1	A	586	SER
1	A	593	PHE
1	A	597	THR
1	A	602	ASP
1	A	606	MET
1	A	609	THR
1	A	631	GLN
1	A	636	PHE
1	A	639	MET
1	A	650	TYR
1	A	651	LEU
1	A	660	THR
1	A	667	LYS
1	A	674	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	678	SER
1	A	688	LEU
1	A	703	HIS
1	A	706	ASP
1	A	707	ASP
1	A	723	LEU
1	A	741	LEU
1	A	762	THR
1	A	793	THR
1	A	797	LYS
1	A	807	THR
1	A	829	THR
1	A	836	SER
1	A	857	THR
1	A	875	SER
1	A	917	ASP
1	A	920	ARG
1	A	958	LEU
1	A	997	LEU
1	A	1021	LEU
1	B	160	LEU
1	B	165	GLN
1	B	170	THR
1	B	172	VAL
1	B	184	ASN
1	B	201	LEU
1	B	205	TRP
1	B	206	ASN
1	B	220	THR
1	B	233	GLU
1	B	239	TYR
1	B	255	HIS
1	B	259	LEU
1	B	293	GLN
1	B	321	ARG
1	B	339	LEU
1	B	340	ASP
1	B	341	ASP
1	B	355	SER
1	B	369	LEU
1	B	376	THR
1	B	383	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	394	LEU
1	B	433	TRP
1	B	435	LEU
1	B	436	LEU
1	B	454	ASP
1	B	468	HIS
1	B	477	MET
1	B	485	LEU
1	B	489	PHE
1	B	497	SER
1	B	501	ILE
1	B	526	SER
1	B	568	PHE
1	B	593	PHE
1	B	598	ASN
1	B	608	LYS
1	B	613	GLN
1	B	636	PHE
1	B	637	LEU
1	B	648	THR
1	B	650	TYR
1	B	653	HIS
1	B	654	ILE
1	B	668	TYR
1	B	681	ILE
1	B	688	LEU
1	B	691	LYS
1	B	723	LEU
1	B	762	THR
1	B	786	ASP
1	B	789	SER
1	B	791	LEU
1	B	798	LEU
1	B	801	ASN
1	B	807	THR
1	B	809	THR
1	B	829	THR
1	B	871	ASP
1	B	915	ASN
1	B	953	VAL
1	B	962	THR
1	B	972	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	973	LEU
1	B	977	LYS
1	B	991	SER
1	B	992	GLU
2	D	4	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	631	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	4L8	C	2	2	6,7,9	0.76	0	7,8,11	1.03	0
2	4L8	D	2	2	6,7,9	0.78	0	7,8,11	1.01	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4L8	C	2	2	-	0/4/6/10	0/0/0/0
2	4L8	D	2	2	-	0/4/6/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	4L8	O-C-CA	-2.03	120.76	125.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	4L8	1	0
2	D	2	4L8	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	1102	1,4	14,14,15	0.57	0	15,19,21	0.50	0
4	NAG	A	1103	4	14,14,15	0.21	0	15,19,21	0.28	0
4	NAG	A	1104	1	14,14,15	0.36	0	15,19,21	0.53	0
4	NAG	A	1105	1	14,14,15	0.31	0	15,19,21	0.39	0
4	NAG	A	1106	1,4	14,14,15	0.32	0	15,19,21	0.31	0
4	NAG	A	1107	4	14,14,15	0.23	0	15,19,21	0.27	0
4	NAG	A	1108	1	14,14,15	0.28	0	15,19,21	0.27	0
4	NAG	A	1109	1	14,14,15	0.39	0	15,19,21	0.42	0
4	NAG	A	1110	1	14,14,15	0.99	1 (7%)	15,19,21	0.77	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1111	1	14,14,15	0.19	0	15,19,21	0.33	0
4	NAG	A	1112	1,4	14,14,15	0.55	0	15,19,21	0.65	0
4	NAG	A	1113	5,4	14,14,15	0.30	0	15,19,21	0.44	0
5	MAN	A	1114	4	11,11,12	0.66	0	15,15,17	1.07	2 (13%)
4	NAG	A	1115	1	14,14,15	0.61	0	15,19,21	0.71	1 (6%)
4	NAG	A	1116	1,4	14,14,15	0.34	0	15,19,21	0.45	0
4	NAG	A	1117	4	14,14,15	0.22	0	15,19,21	0.28	0
4	NAG	B	1102	1	14,14,15	0.19	0	15,19,21	0.37	0
4	NAG	B	1103	1,4	14,14,15	0.35	0	15,19,21	0.50	0
4	NAG	B	1104	4	14,14,15	0.26	0	15,19,21	0.28	0
4	NAG	B	1105	1	14,14,15	0.21	0	15,19,21	0.38	0
4	NAG	B	1106	1	14,14,15	0.26	0	15,19,21	0.36	0
4	NAG	B	1107	1	14,14,15	0.26	0	15,19,21	0.35	0
4	NAG	B	1108	1	14,14,15	0.62	0	15,19,21	0.90	2 (13%)
4	NAG	B	1109	-	14,14,15	0.22	0	15,19,21	0.28	0
4	NAG	B	1110	1	14,14,15	0.87	2 (14%)	15,19,21	0.82	1 (6%)
4	NAG	B	1111	1,4	14,14,15	0.44	0	15,19,21	0.74	1 (6%)
4	NAG	B	1112	4	14,14,15	0.25	0	15,19,21	0.32	0
4	NAG	B	1113	1	14,14,15	0.27	0	15,19,21	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1102	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1103	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1104	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1105	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1106	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1107	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1108	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1109	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1110	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1111	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1112	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1113	5,4	-	0/6/23/26	0/1/1/1
5	MAN	A	1114	4	-	0/2/19/22	0/1/1/1
4	NAG	A	1115	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1116	1,4	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1117	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1102	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1103	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1104	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1105	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1106	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1107	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1108	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1109	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1110	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1111	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1112	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1113	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1110	NAG	C1-C2	2.09	1.55	1.52
4	B	1110	NAG	O5-C1	2.42	1.47	1.43
4	A	1110	NAG	O5-C1	2.88	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1114	MAN	O2-C2-C3	-2.09	105.98	110.19
4	B	1108	NAG	C2-N2-C7	2.15	125.90	123.11
4	A	1115	NAG	C1-O5-C5	2.26	115.46	112.14
5	A	1114	MAN	C1-O5-C5	2.28	115.49	112.14
4	B	1111	NAG	C1-O5-C5	2.33	115.57	112.14
4	A	1110	NAG	C1-O5-C5	2.52	115.84	112.14
4	B	1108	NAG	C1-O5-C5	2.62	116.00	112.14
4	B	1110	NAG	C1-O5-C5	3.00	116.55	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1108	NAG	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1113	NAG	1	0
5	A	1114	MAN	1	0
4	B	1102	NAG	1	0
4	B	1106	NAG	1	0
4	B	1107	NAG	1	0
4	B	1108	NAG	1	0
4	B	1111	NAG	1	0
4	B	1112	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	859/912 (94%)	0.21	25 (2%) 55 54	67, 110, 174, 207	3 (0%)
1	B	852/912 (93%)	0.26	53 (6%) 24 23	73, 147, 195, 229	1 (0%)
2	C	8/10 (80%)	0.07	0 100 100	119, 158, 174, 177	0
2	D	3/10 (30%)	1.45	1 (33%) 0 1	162, 162, 177, 180	0
All	All	1722/1844 (93%)	0.23	79 (4%) 36 35	67, 130, 190, 229	4 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	7.0
1	B	221	PHE	6.6
1	B	622	GLN	5.2
1	B	419	LEU	4.3
1	B	220	THR	4.3
1	B	251	LEU	4.2
1	B	361	PHE	4.1
1	A	207	ILE	4.1
1	B	530	ILE	4.0
1	B	249	GLU	3.9
1	B	250	ALA	3.9
1	A	200	ALA	3.7
1	B	328	LEU	3.7
1	B	209	LEU	3.6
1	B	363	VAL	3.6
1	B	701	ILE	3.5
1	B	702	VAL	3.5
1	B	480	TRP	3.4
1	B	362	ILE	3.4
1	B	627	GLU	3.3
1	B	483	LEU	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	378	VAL	3.3
1	B	619	VAL	3.3
1	A	219	VAL	3.2
1	B	417	LEU	3.2
1	A	234	ILE	3.1
1	B	382	ALA	3.1
1	A	206	ASN	3.1
1	B	306	PHE	3.0
1	A	159	LYS	2.9
1	B	412	TYR	2.9
1	A	386	LYS	2.8
1	B	621	VAL	2.8
1	B	244	ALA	2.7
1	A	334	LYS	2.7
1	B	629	PHE	2.7
1	B	289	PHE	2.7
1	A	208	ILE	2.7
1	A	202	GLN	2.6
1	B	970	SER	2.5
1	A	363	VAL	2.5
2	D	5	HIS	2.5
1	A	245	ILE	2.5
1	A	417	LEU	2.5
1	A	250	ALA	2.4
1	B	257	TYR	2.4
1	B	683	LEU	2.4
1	A	232	ALA	2.4
1	B	319	ILE	2.4
1	A	750	PHE	2.4
1	B	296	PRO	2.4
1	B	736	PHE	2.3
1	A	382	ALA	2.3
1	B	713	ILE	2.3
1	B	823	LEU	2.3
1	B	703	HIS	2.3
1	B	590	TRP	2.3
1	A	185	LEU	2.3
1	B	660	THR	2.3
1	B	540	ILE	2.3
1	A	362	ILE	2.3
1	B	688	LEU	2.2
1	B	326	THR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	234	ILE	2.2
1	A	289	PHE	2.2
1	A	692	VAL	2.1
1	B	691	LYS	2.1
1	A	236	GLU	2.1
1	A	249	GLU	2.1
1	A	355	SER	2.1
1	B	700	TYR	2.1
1	B	381	TYR	2.1
1	B	364	GLY	2.1
1	B	484	TRP	2.1
1	B	365	GLU	2.1
1	B	258	THR	2.1
1	B	436	LEU	2.1
1	B	623	LYS	2.0
1	B	420	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	4L8	D	2	8/10	0.91	0.48	-	132,140,160,168	0
2	4L8	C	2	8/10	0.95	0.33	-	104,114,123,131	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	1113	14/15	0.55	0.41	7.98	165,177,184,186	0
3	ZN	A	1101	1/1	0.99	0.23	0.81	86,86,86,86	0
4	NAG	B	1102	14/15	0.56	0.25	0.09	170,182,187,190	0
3	ZN	B	1101	1/1	0.96	0.21	-0.13	124,124,124,124	0
4	NAG	A	1112	14/15	0.88	0.20	-0.17	123,135,151,156	0
4	NAG	A	1102	14/15	0.90	0.17	-0.67	155,163,177,178	0
4	NAG	B	1103	14/15	0.90	0.17	-2.21	202,206,214,214	0
4	NAG	A	1116	14/15	0.80	0.17	-	197,213,217,222	0
4	NAG	A	1115	14/15	0.84	0.21	-	153,169,176,176	0
4	NAG	B	1107	14/15	0.83	0.18	-	195,199,205,206	0
4	NAG	A	1110	14/15	0.56	0.51	-	140,159,163,166	0
4	NAG	A	1109	14/15	0.78	0.25	-	147,182,193,194	0
4	NAG	A	1111	14/15	0.71	0.24	-	125,143,161,167	0
4	NAG	B	1106	14/15	0.81	0.31	-	186,197,204,204	0
4	NAG	A	1105	14/15	0.86	0.18	-	179,190,197,204	0
4	NAG	A	1113	14/15	0.89	0.17	-	137,145,164,165	0
4	NAG	A	1117	14/15	0.64	0.27	-	202,211,217,218	0
4	NAG	B	1104	14/15	0.82	0.23	-	202,208,214,215	0
4	NAG	A	1104	14/15	0.79	0.20	-	174,182,185,187	0
4	NAG	B	1105	14/15	0.79	0.23	-	174,186,192,193	0
4	NAG	A	1108	14/15	0.76	0.26	-	151,156,172,176	0
4	NAG	B	1112	14/15	0.73	0.32	-	188,194,203,206	0
4	NAG	B	1108	14/15	0.88	0.20	-	171,178,184,185	0
4	NAG	B	1109	14/15	0.78	0.19	-	161,173,182,184	0
4	NAG	B	1110	14/15	0.77	0.28	-	165,180,191,193	0
4	NAG	A	1103	14/15	0.84	0.23	-	161,176,182,184	0
4	NAG	A	1107	14/15	0.67	0.30	-	179,203,212,213	0
5	MAN	A	1114	11/12	0.77	0.26	-	175,182,189,211	0
4	NAG	A	1106	14/15	0.83	0.22	-	167,177,196,196	0
4	NAG	B	1111	14/15	0.73	0.24	-	169,181,188,191	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.